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MECHANISMS OF EXHAUST POLLUTANTS AND PLUME FORMATION IN CONTINU--ETC(U)
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MECHANISMS OF EXHAUST POLLUTANTS AND PLUME FORMATION IN CONTINUOUS COMBUSTION

(AFOSR 74-2710)

FINAL REPORT

G.S. Samuelsen
R.M. Hamberg

UCI-ARTR-78-2

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MECHANISMS OF EXHAUST POLLUTANTS AND PLUME FORMATION IN CONTINUOUS COMBUSTION

(AFOSR 74-2710)

Summary of Progress

1 May 1974 to 28 February 1978

An analytical and experimental study has been conducted to promote an understanding of the processes governing the emission characteristics of continuous combustion power sources. The study addressed the development and assessment of numerical codes for backmixed flows, the formation of pollutants in backmixed flows, and questions associated with sampling oxides of nitrogen.

Specification of eddy viscosity was found to have the greatest impact on numerical code performance. However, it was shown to be first necessary to insure that other elements of the model (*e.g.* boundary conditions and grid specification) are in order. Laser Doppler Anemometry was developed for the measurement of velocity and turbulence intensity.

The pollutant formation studies employed an aerodynamic flameholder to explore the extended lean equivalence ratios made available by fuel-enriched jet flow. The net effect was a substantial reduction in nitrogen oxides emissions.

Reduction of NO_2 to NO and removal of NO_x were the dominant changes identified under conditions simulating sample line environments.

MECHANISMS OF EXHAUST POLLUTANTS AND PLUME FORMATION IN CONTINUOUS COMBUSTION

(AFOSR 74-2710)

1.0 Introduction

The AFOSR program conducted at the UCI Combustion Laboratory has been directed to modeling and exploring mechanisms associated with pollutant production in continuous combustion. The objectives of the study were:

- To develop and verify numerical methods and associated submodels of turbulence and kinetics as applied to recirculating turbulent reacting flowfields characteristic of turbine combustion via a judicious coupling of numerical methods to experiment. Such information is pertinent to establishing a method that can be readily adapted to the flow geometry of gas turbine, dump, and ramjet combustors.

- To develop an understanding of pollutant formation in continuous combustion stabilized by recirculation. Such information is pertinent to reducing environmental impact and controlling plume signature.

- To initiate and/or conduct supplemental studies pertinent to pollutant formation, combustion stability, and use of alternative fuels in turbine, dump, and ramjet combustors.

To address these objectives, the AFOSR UCI Combustion Laboratory program has included both experimental and analytical studies in a task organization structure which evolved into three elements:

- <u>Element A: Model Development and Evaluation</u>

  The evaluation and refinement of numerical procedures by a judicious comparison of numerically predicted profiles of velocity, turbulence energy, temperature, tracer concentration, and mass fractions of hydrocarbon | nitric oxide, nitrogen dioxide, carbon monoxide, oxygen and carbon dioxide to experimentally determined profiles.

- <u>Element B: Mechanisms of Pollutant/Plume Formation</u>

  The conduct of parametric studies to identify the relative contribution of the chemical reactions, transport processes, and system parameters to pollutant formation.

- **Element C: Supplemental Studies**

  The initiation and/or conduct of the following studies that support the investigations of combustion stability, pollutant formation, and numerical methods, and address specialized questions current to practical backmixed combustion systems:

  NO Probe. The initiation and conduct of a study to explore chemical transformations of nitrogen oxides in sample probes and sample lines while sampling combustion products.

  Particulate Formation/Luminosity. The initiation of a study to explore (1) particulate formation in backmixed combustion with special emphasis on broad specification fuels, and (2) luminous flame radiation in backmixed combustion with special attention to broad specification fuels and impact on combustor linear degradation.

  Center-Body Stabilized Premixed and Nonpremixed. The initiation of a study to address numerical method development and evaluation, and pollutant formation in recirculating, center-body stabilized flows operating in both premixed and nonpremixed modes.

  Limits of Combustion. The initiation of a study to assess the behavior of the backmixed region and pollutant formation that accompany flame instability at blowout.

The recirculating flow combustor employed in the UCI program is the opposed-jet combustor (OJC) shown in schematic in Figure 1. The system features a wide range of operating conditions made possible by modest changes in the jet velocity and jet mixture ratio. As a result, numerical methods can be challenged and pollutant formation explored over a wide range of flow encounters. The combustor was operated at atmospheric pressure with a preheat capability to 350°C (expandable to 600°C).

Gaseous combustion product sampling was conducted with water cooled probes. Local measurement of velocity and turbulence intensity was conducted with laser velocimetry. A detailed description of the combustor facility is provided elsewhere (Peterson, 1976a).

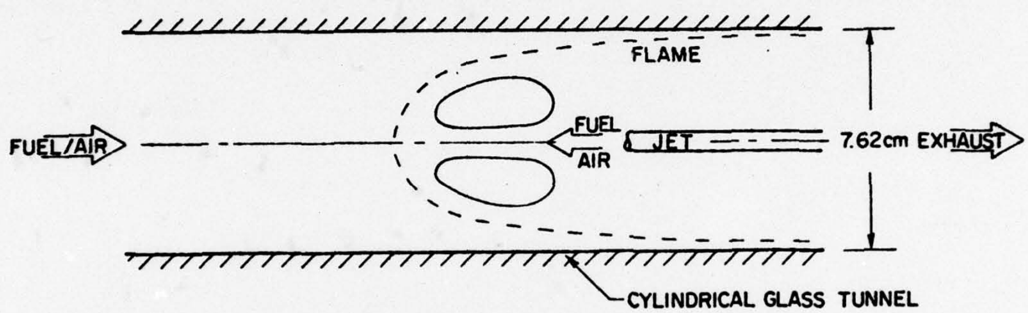

Figure 1 **Opposed Jet Combustor (OJC)**

2.0 Description of Results

Descriptions of the research results are presented for each element below. A statement of future direction accompanies each summary as appropriate. The supporting documentation for each research result is referenced as a paper presented, publication and/or report where available. A listing of the papers presented, publications and reports are presented in Tables I, II, and III respectively.

Element A: Model Development and Evaluation

Goal. The goal of this element was to develop and evaluate predictive models with emphasis on the specification of eddy viscosity, computational grid dimensions, and inlet and boundary conditions.

Results. Studies conducted to compare numerically generated predictions of pollutant formation to experimental measurements have demonstrated that elliptic models are capable of predicting general trends but are not capable of providing the detail necessary to the prediction of pollutant behavior (Wuerer, 1976; Peck and Samuelsen, 1975; Peck and Samuelsen, 1977a). As a result, studies were initiated to assess the ability of the elliptic models to correctly predict mass and momentum transport in nonreacting flowfields into which a CO tracer is introduced.

In the initial study (Peck, 1976; Peck and Samuelsen, 1977b; Peck and Samuelsen, 1977c); the relative merits of a zero-equation and a two-equation eddy viscosity submodel for simulating turbulence transport properties in recirculating flows was assessed by comparing continuum model predictions of the turbulent, backmixed flowfield to experimental measurements.

Both eddy viscosity models qualitatively described the bulk hydrodynamic flowfield, but the detailed flow structure was inadequately represented. Mass transport estimates based on the zero-equation viscosity model conformed favorably to experiment. The two-equation turbulence submodel yielded consistently poor correlation. The deficiency of the two-equation eddy viscosity model predictions was attributed to the boundary condition specification for the turbulence energy dissipation rate. It was shown that the turbulence energy dissipation rate adjacent to critical solid walls strongly influenced the overall mixing characteristics of the two-equation submodel.

The results indicated that the zero-equation eddy viscosity model provided cost-effective predictions of the general fluid flow patterns and mass transport trends in turbulent, confined flows exhibiting strong recirculation. The two-equation eddy viscosity submodel provided better resolution of small-scale turbulence processes, but required careful testing to ensure realistic predictions.

In a second study (Wuerer and Samuelsen, 1977), the sensitivity of the predicted flowfield structure to the specification of eddy viscosity, computational grid dimensions, and inlet boundary conditions were considered. Specification of the eddy viscosity was found to have the greatest impact. The results indicated that a viscosity model capable of providing a spatially varying description of turbulence generation and dissipation is essential in order to obtain a realistic solution. A two-equation k-ϵ model demonstrated promise in providing the required detail. Precautions were shown to be warranted in the use of the model to describe the important features of the flowfield. Calibration of the constants in the model was one approach identified to remedy the observed discrepancies. However, it was shown to be first necessary to insure that other elements of the model (*e.g.* boundary conditions and grid specification) are in order.

Direction. Studies are in progress to collect and compare LDA data to local distributions of velocity and turbulence intensity predicted numerically. The development of the LDA system is described under Element B.

A second combustor configuration, the center body combustor (CBC), is being employed as well. The CBC, shown in Figure 2, is scaled from the Air Force Aero Propulsion Laboratory (AFAPL) combustor planned for computer model evaluation. The CBC will offer the advantages of similarity with the AFAPL combustor, operation in both the premixed and nonpremixed mode (see Element C), and more effective representation of practical combustor concepts. In addition, the streamline enveloping the recirculation region has one point of attachment in contrast to the OJC which has none. The CBC will also resolve shortcomings of the OJC which may reduce its effectiveness as a model combustor for backmixed flow studies. LDA data and time lapse photography indicate that the backmixed region of the OJC has large scale instabilities which may compromise (1) LDA measurements within the recirculation zone, and (2) application of time averaged modeling. In addition, the high velocity and small issuing diameter of the jet place a strain on the computational method which, while interesting to unravel, are not representative of practical systems.

In other studies presently in progress, experimental data are being collected for the heated (no reaction, air preheat) and hot (reaction) flow conditions. A complementary, two (expandable to three) year National Science Foundation program has been awarded to address the modeling of a critical part of the predictive method--the direct influence of turbulence on the kinetic rate of reactions.

Element B: Mechanisms of Pollutant/Plume Formation

Goal. The goal of this element was to evaluate the emission characteristics of gaseous-fueled, recirculating flow combustion.

Results. The study included the development of a laser Doppler Anemometer (LDA) system for the measurement of local velocity and turbulence intensity, and an experimental investigation of the lean stabilized emission behavior of the opposed jet combustor.

The LDA system was developed to measure a single component of velocity including frequency shifting. This capability includes the measurement of both local velocity and turbulence intensity. Such measurements are intended to characterize the local fluid behavior as one element of the pollutant formation mechanics.

The key accomplishments of the LDA development were:

Equipment Development

- Evaluation of the DISA piezo-electric frequency shift device
- Evaluation of Macrodyne Counter Processor
- Acquisition of a rotating grating frequency shift device
- Acquisition of an amplifier for the Photomultiplier output
- Fabrication of an optical system for the rotating grating
- Development of velocity data reduction software for the PDP-11 computer
- Evaluation of the signal response for latex versus salt particles

Flow Field Measurements

- Validation of the LDA measurements against pitot measurements
- Validation of frequency shift
- Acquisition of combustor inlet velocity and turbulence intensity measurements to provide boundary conditions for the flow analysis
- Acquisition of combustor flowfield velocity measurements to define the influence of the opposed jet and recirculation zone on local velocity and turbulence intensity.

The experimental investigation (Peterson 1976b; Peterson and Samuelsen, 1977; Peterson and Samuelsen, 1978) explored the emission behavior of aerodynamically stabilized, lean premixed combustion. Exit plane profiles of temperature and pollutant species concentration were examined for a propane/air fired opposed jet combustor. Results for a range of lean combustion conditions indicated that lean operation significantly reduces the emission of nitrogen oxides and carbon monoxide from levels measured at stoichiometric operation. Hydrocarbon emission increases. For main stream equivalence ratios between 0.8 and 1.0, the emission behavior was explained by reactions occurring in both the stabilization zone and the region downstream. Below a main stream equivalence ratio of 0.8, reaction downstream of the stabilization zone was suppressed, and the emission behavior was altered. Enrichment of the jet flameholder at a given main stream equivalence ratio did not significantly affect total pollutant emission. However, jet enrichment allowed stabilization of leaner main stream mixtures than allowed with bluff body or sudden expansion flameholders. This study not only characterized the emission behavior of the aerodynamic flameholder, but served as the foundation for the pollutant mechanics study as well.

Direction. Two studies are in progress in support of the pollutant mechanics element. In one, the flowfield of the combustor is being mapped for temperature, velocity, turbulence intensity, and species composition for a variety of flow conditions. In the second study, the effect of inlet turbulence intensity on emission behavior is being assessed. The LDA is presently being used to characterize the local velocity and turbulence intensity of the OJC, and will be used to characterize the local velocity and turbulence intensity of the center body combustor under development (as described under Element C).

Element C: Supplemental Studies

Three supplemental studies have been initiated as part of the AFOSR program in anticipation of developing Air Force needs. For two of the studies (NO Probe, Particulate Formation/Luminosity), additional funding has been obtained or requested from the AFOSR and non-AFOSR sources as indicated below. The third study (premixed and nonpremixed) will strengthen both the continuation of the AFOSR program and the particulate formation/luminosity study for which complementary funding is being sought.

NO PROBE

Goal. The goal of this supplemental study was to initiate and conduct an investigation that explored the types and extent of transformations of nitrogen oxides in sample probes and sample lines in the presence of oxidizing and reducing species, and to identify the conditions under which transformations can occur.

Results. Nitrogen oxides are especially susceptible to chemical change in sample probes and sample lines. To assess measurement errors that may be encountered when sampling nitrogen oxides, concentration changes were measured across two-meter lengths of 316 stainless steel and silica tubing. The combustion products entering the tubes were simulated (12% CO_2, 500 ppm NO, 75 ppm NO_2, variable O_2, CO, H_2, and HC, balance N_2). The tubing was maintained isothermally at select temperatures in the range of 25°C to 400°C. The results were reported in four papers (Samuelsen and Harman, 1975; Benson, Samuelsen, and Peck, 1976; Benson and Samuelsen, 1976; Benson and Samuelsen, 1977), two publications (Samuelsen and Harman, 1977; Benson and Samuelsen, 1978), and one report (Benson, 1978).

Overall, transformation was more pronounced in stainless steel than silica. Reduction of NO_2 to NO, and removal of NO_2 and NO were the dominant transformations observed. In the presence of reactive reducing species (*e.g.* 500 ppm ethylene or propylene), reduction of NO_2 to NO occurred as low as 200°C in stainless steel and 400°C in silica. Removal of NO_x was observed in the absence of oxygen at 400°C in stainless steel. In the presence of less reactive reducing species (*e.g.* methane and carbon monoxide), either higher concentrations or higher temperatures were required to reduce NO_2 to NO. The presence of oxygen suppressed but did not prevent the reduction of NO_2 to NO. Neither methane nor carbon monoxide were active in removing NO_x. The data were collected in the pressure range of 1.0 to 1.15 atmospheres.

Direction. The experiment is being expanded to include water in the simulated combustion products and to provide a flat flame burner as a bridge between the simulated combustion products and conditions encountered in practical applications. Under complementary funding from the Civil and Environmental Engineering Development Office (CEEDO), the maximum temperature will be elevated, the effects of residence time, pressure, and probe conditioning will be assessed, and a review of the turbine emission data will be conducted.

A proposal is outstanding to the Naval Air Propulsion Center for a program to simulate the tip of hot sample probes and assess the transformations that may occur under such conditions.

Particulate Formation/Luminosity

Goal. The goal of this supplemental study was to initiate an investigation of soot formation and burnout in recirculating flows for proposed broad specification fuels.

Results. Designs for liquid-fuel operation and luminosity detection were completed.

Direction. The facility will provide experimental data necessary to support future efforts in the AFOSR program which address modeling of radiation and soot formation and burnout.

A separate application is in preparation for funding the measurement of local particle size and concentration using optical methods. The program is joint with Spectron Development Laboratories.

Center-Body Stabilized Premixed and Nonpremixed Operation

Goal. The goal of this supplemental study was to develop the capability for numerical method development and evaluation, and pollutant formation studies in recirculating, center-body stabilized flows operating in either a premixed or nonpremixed mode.

Results. Designs have been completed for premixed fuel preparation, and premixed and nonpremixed center-body stabilized combustion. The center-body combustor (CBC), shown in Figure 2, is a scaled version of the AFAPL combustor designed for evaluation of the computer code GFREP.

The capability of premixed-nonpremixed center body stabilized combustion is an appropriate step to complement the OJC, and will provide an important experiment for the development of models and exploration of pollutant formation mechanics in gas turbine combustor type combustion.

As previously discussed, the CBC will not only offer a configuration more representative of practical combustor concepts, but will provide an alternative to the challenges (flow stability, and a small diameter high velocity jet) encountered in modeling the OJC and collecting OJC LDA measurements.

Limits of Combustion

Goal. The goal of this supplemental study was to initiate an investigation designed to evaluate the backmixed zone characteristics (size, velocity distribution, turbulence intensity) and emission behavior that accompany flame instability at blowout.

Results. The development and application of the LDA has provided measurements of the combustor flowfield velocity, and defined the influence of the opposed jet and recirculation zone on local velocity and turbulence intensity. In addition, preliminary applications of high speed photography have identified a large degree of oscillitory and unsteady motion in and about the backmixed zone.

Direction. The existing LDA system is limited to measurements outside the backmixed zone. The system is being expanded to allow the capability of velocity and turbulence intensity measurements at the limits of combustion and within the backmixed region. In addition, Schlieren optical test methods are presently being designed for use in tracking the flow patterns in the backmixed region.

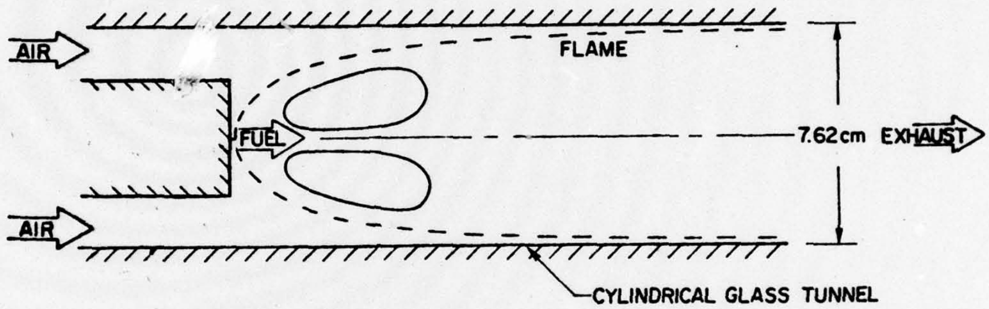

Figure 2 Center Body Combustor (CBC)

TABLE I

Papers Presented

ELEMENT	TITLE	LOCATION
A. Model Development and Evaluation	Peck, R.E., Samuelsen, G.S. (1975) Analytical and Experimental Study of Turbulent Methane-Fired Backmixed Combustion	AIAA/SAE 11th Propulsion Conference Anaheim, California
	Peck, R.E., Samuelsen, G.S. (1977g) Eddy Viscosity Modeling in the Prediction of Turbulent Backmixed Combustion Performance	Sixteenth (International) Symposium on Combustion
	Wuerer, J.E., Samuelsen, G.S. (1977) Mass and Momentum Transport in Turbulent Flow with Backmixing	1977 Fall Meeting Western States Section/Combustion Institute Stanford University
B. Mechanisms of Pollutant/Plume Formation	Peterson, P.R., Samuelsen, G.S. (1977) Emission Behavior of Aerodynamically Stabilized Lean Premixed Combustion	1977 Spring Meeting Western States Section/Combustion Institute, *University of Washington*
C. Supplemental Studies	Harman, J.N. III, Samuelsen, G.S. (1975) Transformation of Oxides of Nitrogen while Sampling Combustion Products	First International Chemical Congress ACS, Mexico City
	Benson, R.C., Samuelsen, G.S., Peck, R.E. (1976) Oxides of Nitrogen Transformation While Sampling Combustion Products Containing Carbon Monoxide	1976 Spring Meeting Western States Section/Combustion Institute University of Utah
	Benson, R.C., Samuelsen, G.S. (1976) Oxides of Nitrogen Transformation While Sampling Combustion Products Containing Carbon Monoxide and Hydrogen	1976 Fall Meeting Western States Section/Combustion Institute University of California, San Diego
	Benson, R.C., Samuelsen, G.S. (1977) Oxides of Nitrogen Transformation While Sampling Combustion Products Containing Carbon Monoxide, Hydrogen, and Hydrocarbons	1977 Spring Meeting Western States Section/Combustion Institute, University of Washington

TABLE II

Publications

ELEMENT	TITLE	SOURCE
A. Model Development and Evaluation	Peck, R.E.,Samuelsen, G.S. (1977a) Analytical and Experimental Study of Turbulent Methane Fired Backmixed Combustion	AIAA Journal - May 1977 Vol. 15, No. 5, pp 730-732
	Peck, R.E., Samuelsen, G.S. (1977c) Eddy Viscosity in the Prediction of Turbulent Backmixed Combustion Performance	Sixteenth (International) Symposium on Combustion, pp 1675-1687
B. Mechanisms of Pollutant/Plume Formation	Peterson, P.R., Samuelsen, G.S. (1978) Emission Behavior of Aerodynamically Stabilized, Lean Premixed Combustion	Combustion Science and Technology (submitted)
C. Supplemental Studies	Harman, John N., III, Samuelsen, G.S. (1977) Chemical Transformations of Nitrogen Oxides While Sampling Combustion Products	Journal of Air Pollution Control Association July 1977, Vol. 27, No. 7 pp 648-655
	Benson, R.C., Samuelsen, G.S. (1978) Transformation of Nitrogen Oxides While Sampling Combustion Products in the Presence of Oxygen, Carbon Monoxide, and Hydrocarbons	Combustion & Flame (submitted)

TABLE III

Air Resources Technical Reports

ELEMENT	TITLE	SOURCE
A. Model Development and Evaluation	Peck, R.E. (1976) Eddy Viscosity Modeling in the Prediction of Combustion-Chamber Flows	UCI Combustion Laboratory UCI-ARTR-76-12
	Wuerer, J.E. (1976) Flowfield Predictions of an Opposed Reacting Jet Combustor	UCI Combustion Laboratory UCI-ARTR-76-8
B. Mechanisms of Pollutant Plume Formation	Peterson, P.R. (1976a) Opposed Jet Combustor Experimental Facility	UCI Combustion Laboratory UCI-ARTR-76-14
	Peterson, P.R. (1976b) System Design and Evaluation to Assess Air Preheat Effects on Emissions from an Atmospheric Combustor	UCI Combustion Laboratory UCI-ARTR-76-13
C. Supplemental Studies	Benson, R.C. (1978) Experimental Assessment of Nitrogen Oxides Transformations While Sampling Combustion Products	UCI Combustion Laboratory UCI-ARTR-78-1

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

An analytical and experimental study has been conducted to promote an understanding of the processes governing the emission characteristics of continuous combustion power sources and thus provide a basis for reducing adverse environmental effects and for controlling plume signatures resulting from aircraft operation. The study addressed the development and assessment of numerical codes for backmixed flows, the formation of pollutants in backmixed flows, and questions associated with sampling oxides of nitrogen. The backmixed flow selected for study was the opposed jet laboratory combustor (OJC). The system features a wide range of operating conditions made possible by modest changes

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SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered) in the jet velocity and mixture ratio. As a result, numerical models can be challenged and pollutant formation explored over a wide range of flow encounters. Two numerical methods were used for modeling purposes. The work included both reacting and non-reacting flow, but emphasized the utility and range of applicability of the numerical methods for the case of isothermal flow. Eddy viscosity models, inlet and boundary condition specification, and grid sizing were addressed in a series of systematic tests of prediction against experiment. Specification of eddy viscosity was found to have the greatest impact in numerical performance. However, it was shown to be first necessary for other elements of the model (e.g. boundary conditions and grid specification) to be in order. Laser Doppler Anemometry was developed for the measurement of velocity and turbulence intensity. The pollutant formation studies addressed the lean stabilized combustion characteristics of the OJC aerodynamic flameholder. The emission behavior was explored at expended lean equivalence ratios produced by fuel-enriched jet flow. The net effect was a substantial reduction in nitrogen oxides emission. The combustion sampling work focused on the change to nitrogen dioxide (NO_2) and nitric oxide (NO) concentrations in mixtures representative of combustion products: oxygen, coarbon monoxide, methane, ethylene, hydrogene, propylene, carbon dioxide and nitrogen. Stainless steel and silica $\frac{1}{4}$-inch tubes were evaluated. Reduction of NO_2 to NO and the removal of NO_x were the dominant changes observed. The extent of chemical change and the conditions for which chemical changes occurs were identified over the temperature range 25^o to 400^oC.